

Oral presentation

Crystal structures of moderately complex organic molecules are predictable

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A comprehensive computational strategy for the prediction of crystal structures is presented that has scored an unprecedented 4 in 4 success rate at the 2007 international Crystal-Structure Prediction Blind Test [1]. Key components of the new approach, implemented in the GRACE software package, are a dispersion-corrected Density Functional Theory (DFT) method developed in-house for the accurate calculation of lattice energies [2], a robust procedure for the parameterisation of non-transferable force fields on a per molecule basis [2], and a novel approach for crystal-structure generation. The dispersion-corrected DFT method combines DFT calculations by means of the VASP program with an empirical Van der Waals correction; it is used for the final lattice energy ranking and acts as a reference standard for force-field parameterisation. A tailor-made force field is derived for each molecule to be considered and used for crystal-structure generation as well as for the preparation of second derivative matrices for the final lattice-energy optimisations with the dispersion-corrected DFT method. Based on the known statistical deviation between the tailor-made force field and the dispersion-corrected DFT method, it is possible to select a shortlist of crystal structures from a small energy window for the final lattice-energy optimisations and ranking of the predicted crystal structures with the dispersion-corrected DFT method. In addition to the Blind Test results, validation studies for 15 organic molecules are presented, including ethane, ethylene, acetylene, methanol, urea, acetic acid, cyclohexane-1,4-dione, paracetamol, previous Blind Test molecules I to VI and a pharmaceutical compound for which crystal structures have been predicted in a blind test fashion. 17 out of the 18

experimentally observed crystal forms of these molecules are found among the first two most stable predicted crystal structures.

References

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